s5.m15.p14 **The crystal chemistry and morphology of a new arsenate: $Ca_2NaH(AsO_4)_2{\cdot}4H_2O$.** L. Torre-Fernández[2], J. D. Rodríguez[1], M. Prieto[1], A. Jiménez[1] and S. García-Granda[2]. [1]*Dpto. Geología, c/ Jesús Arias de Velasco, s/n, 33005 Oviedo. Spainhttp://geol.uniovi.es/uk/Areas/Cristal/CrystalGrowth.htm.* [2]*Dpto. Química Física y Analítica, c/ Julián Clavería 8, 33006 Oviedo, Spain. E-mail: ltf@fq.uniovi.es*

**Keywords: Arsenate; Morphology**

Crystallization experiments, single crystal X-ray diffraction and SEM studies of $Ca_2NaH(AsO_4)_2{\cdot}4H_2O$, are described. Crystals of this new arsenate were synthesized at 25 ± 0.1 °C by mixing aqueous solutions of $Na_2HAsO_4{\cdot}7H_2O$ (1M) and $CaCl_2$ (0.01M). $Ca_2NaH(AsO_4)_2{\cdot}4H_2O$ crystallises in the triclinic system, space group P-1. The unit-cell parameters are $a_0$ =6.68(2) Å , $b_0$ = 8.223(7) Å, $c_0$ = 12.54(2) Å and α= 73.5(2)°, β= 78.9(1)°, γ= 87.5(1)°, Z = 2, V=647.8 Å$^3$. The crystal structure was solved and the Hydrogen atoms were located and included in the refinement. All atoms of the structure were found to be in general positions.

The structure of $Ca_2NaH(AsO_4)_2{\cdot}4H_2O$ can be described as layers parallel to (001) in which the two crystallographic independent As atoms coordinate with 4 oxygen to form isolated tetrahedron. In the layers, the [$AsO_4$] tetrahedra are joined to [$CaO_6$] octahedron. Sodium is coordinated with six oxygen atoms to form irregular [$NaO_6$] octahedra, which form chains along [010]. The slices of [$AsO_4$] and [$CaO_6$] are linked by [$NaO_6$] octahedra and water molecules.

Representative individuals were selected for the SEM study. Figure 1 shows the typical flaky morphologies of $Ca_2NaH(AsO_4)_2{\cdot}4H_2O$ single crystals. The results of microanalysis reveal that the weights (in atomic percent) of Na (~5%) is half of the amount of As and Ca (~10%).

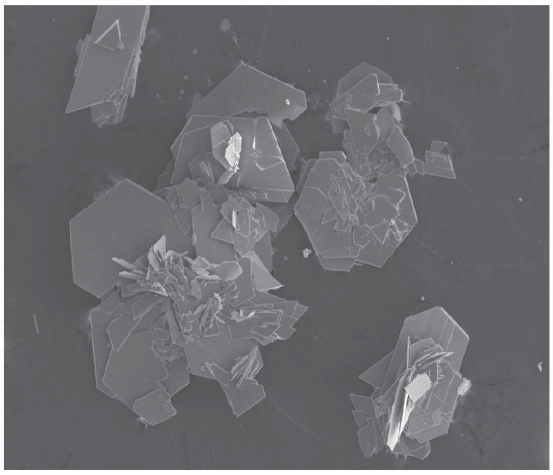

Figure 1: Electron microphotograph of $Ca_2NaH(AsO_4)_2{\cdot}4H_2O$ crystals.

s5.m15.p15 **Absorption and reflectance UV-VIS-IR-spectroscopy application for lattice defects research in diamonds.** M.A. Viktorov, A.S. Marfunin, Y.B. Shelementiev, *Moscow State University, Department of Geology, 119992 Moscow, Russia. E-mail: viktorov@pisem.net*

**Keywords: Diamond; Spectroscopy; Lattice defects**

Several samples of natural and synthetic diamonds were investigated by the means of UV-VIS-IR-range absorption and reflectance spectroscopy (at room temperature). Also electron microscopy, spectral (at liquid nitrogen temperature) cathodeluminescence and color cathodeluminescence were applied to study them.

One of the purposes of the research was to make some correlation between absorption and reflectance spectra in UV-VIS-IR-ranges and to proceed with lattice defects concentration calculation. Other includes investigation of diamond color origin, modeling of structure of some lattice defects in diamonds and modeling of transformational mechanisms of lattice defects during annealing and irradiation processes.

We investigated the collection of several octahedral natural diamond crystals, synthetic diamond crystals, flat plates cut from natural and synthetic diamonds. Several samples (natural octahedral diamond crystal) have undergone annealing at the high temperatures of 1700-1800 degrees C under high pressure (about 6 GPa, during 6 hours), some samples (octahedral natural diamond crystals, natural and synthetic diamond flat plates) were irradiated by protons, several samples undergone color changing to black by new technology at low P-T-parameters. Irradiated samples then were annealed at the different temperatures in the range of 800-900 degrees C during 4-5 hours. Before and after annealing and irradiation spectroscopic data was acquired.

Interpreting of acquired data allows to model structure of some lattice defects in diamond and also provides a useful information on mechanisms of the transformation and stability of lattice defects in diamonds and causes of diamond color.